

# Argonne National Laboratory

A TABULATION OF THE INTERIONIC POTENTIAL  
IN THE ALKALI METALS

by

D. L. Price, Wei-Mei Shyu,  
K. S. Singwi, and M. P. Tosi

The facilities of Argonne National Laboratory are owned by the United States Government. Under the terms of a contract (W-31-109-Eng-38) between the U. S. Atomic Energy Commission, Argonne Universities Association and The University of Chicago, the University employs the staff and operates the Laboratory in accordance with policies and programs formulated, approved and reviewed by the Association.

#### MEMBERS OF ARGONNE UNIVERSITIES ASSOCIATION

The University of Arizona	Kansas State University	The Ohio State University
Carnegie-Mellon University	The University of Kansas	Ohio University
Case Western Reserve University	Loyola University	The Pennsylvania State University
The University of Chicago	Marquette University	Purdue University
University of Cincinnati	Michigan State University	Saint Louis University
Illinois Institute of Technology	The University of Michigan	Southern Illinois University
University of Illinois	University of Minnesota	The University of Texas at Austin
Indiana University	University of Missouri	Washington University
Iowa State University	Northwestern University	Wayne State University
The University of Iowa	University of Notre Dame	The University of Wisconsin

#### NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately-owned rights.

Printed in the United States of America  
Available from  
National Technical Information Service  
U.S. Department of Commerce  
Springfield, Virginia 22151  
Price: Printed Copy \$3.00; Microfiche \$0.65

ARGONNE NATIONAL LABORATORY  
9700 South Cass Avenue  
Argonne, Illinois 60439

A TABULATION OF THE INTERIONIC POTENTIAL  
IN THE ALKALI METALS

by

D. L. Price, Wei-Mei Shyu,  
K. S. Singwi, and M. P. Tosi

Solid State Science Division

November 1970



## TABLE OF CONTENTS

	<u>Page</u>
ABSTRACT . . . . .	5
I. INTRODUCTION. . . . .	5
II. THEORETICAL SCHEME. . . . .	6
III. NUMERICAL VALUES OF THE INTERIONIC POTENTIAL. . . . .	8
REFERENCES . . . . .	17

4

LIST OF TABLES

<u>No.</u>	<u>Title</u>	<u>Page</u>
I.	Values of the Parameters Used in the Calculations . . . . .	7
II.	Interionic Potential for Lithium . . . . .	8
III.	Interionic Potential for Sodium. . . . .	10
IV.	Interionic Potential for Potassium . . . . .	11
V.	Interionic Potential for Rubidium . . . . .	12
VI.	Interionic Potential for Cesium . . . . .	15

A TABULATION OF THE INTERIONIC POTENTIAL  
IN THE ALKALI METALS

by

D. L. Price, Wei-Mei Shyu,  
K. S. Singwi, and M. P. Tosi

ABSTRACT

This report presents a tabulation of the effective interionic potential for the five alkali metals. The potential is based on the self-consistent treatment of correlations in the electron liquid recently given by Singwi, Sjölander, Tosi, and Land (Phys. Rev. B1, 1044 (1970)). A simple form for pseudopotential suggested by Ashcroft (Phys. Lett. 23, 48 (1966)) has been used, in which the only parameter is the core radius. Appropriate values of the core radius have been determined from an analysis of phonon dispersion curves and interatomic force constants. The value for cesium, for which these data do not exist, has been obtained by extrapolation.

I. INTRODUCTION

Recent work of Singwi et al.<sup>1</sup> has presented an improved self-consistent treatment of correlations in the homogeneous electron liquid. This treatment yields a reasonably accurate dielectric function through the whole range of wave vector and electron density of interest in the theory of metals. This screening function has been used<sup>2</sup> in calculations of the lattice dynamics of the alkali metals; good agreement with the phonon dispersion curves, as determined by neutron inelastic scattering experiments, can be obtained with the one-parameter local pseudopotential suggested by Ashcroft,<sup>3</sup> with values for the parameter which are in good agreement (for sodium and potassium) or consistent (for lithium and rubidium) with those derived from Fermi surface and liquid-resistivity data. The results of this analysis have been confirmed by an independent analysis<sup>4</sup> of the force constants for various orders of neighbors in the metal lattice.

This report collects the numerical values of the effective interionic potential as a function of the interionic distance, as obtained from these analyses of phonon data.

## II. THEORETICAL SCHEME

The effective interionic potential is written in the form

$$V(r) = \frac{Z^2 e^2}{r} - \frac{2 Z^2 e^2}{\pi} \int_0^\infty G(q) \frac{\sin(qr)}{qr} dq, \quad (1)$$

where the second term represents the ion-electron-ion contribution. The function  $G(q)$ , introduced by Cochran,<sup>5</sup> is given in the terms of the bare-ion pseudopotential form factor,  $w(q)$ , and of the dielectric function,  $\epsilon(q)$ , as follows:

$$G(q) = \left| \frac{w(q)}{-4\pi Ze^2/\Omega q^2} \right|^2 \left[ 1 - \frac{1}{\epsilon(q)} \right], \quad (2)$$

where  $Z$  and  $\Omega$  are, respectively, the number of conduction electrons and the volume per ion.

We have adopted the analytic form suggested by Ashcroft<sup>3</sup> for the bare-ion pseudopotential,

$$w(q) = -\frac{4\pi Ze^2}{\Omega q^2} \cos(qr_c a_0), \quad (3)$$

where  $r_c$  is an adjustable parameter, representing an effective radius of the ion core. On the other hand, the dielectric function is given by the expression

$$\epsilon(q) = 1 + \frac{\Omega_0(q)}{1 - f(q)\Omega_0(q)}, \quad (4)$$

where  $\Omega_0(q)$  is the Lindhard electron polarizability times  $(-4\pi e^2/q^2)$ ,

$$\Omega_0(q) = \frac{k_F^2 T}{q^2} F(q/k_F), \quad (5)$$

with

$$F(x) = \frac{1}{2} + \frac{4-x^2}{8x} \ln \left| \frac{2+x}{2-x} \right| \quad (6)$$

and

$$k_F^2 T = \frac{m^*}{m} \frac{4k_F}{\pi a_0}. \quad (7)$$

Here,  $k_F$  is the Fermi momentum; band-structure effects on the conduction electrons have been included solely by introducing an effective mass  $m^*$ .

The function  $f(q)$  in Eq. 4 accounts for exchange and correlation effects among the conduction electrons; it has been evaluated by Singwi *et al.*<sup>1</sup> in a self-consistent treatment, and is well represented by the analytic form

$$f(q) = A \{1 - \exp[-B(q/k_F)^2]\}. \quad (8)$$

The constants  $A$  and  $B$  have a weak dependence on the density parameter  $r_s$ , defined by

$$\Omega/Z = \frac{4\pi}{3} r_s^3 a_0^3. \quad (9)$$

These parameters are tabulated for integral  $r_s$  in Ref. 1, and the values appropriate for the relevant value of

$$r_s^* = \frac{m^*}{m} r_s$$

have been obtained by interpolation.

Table I reports, from Refs. 2 and 4, the values of the parameters used in the analysis of the phonon data. The values for the effective mass  $m^*$  were taken from published band-structure calculations. For lithium, rubidium, and cesium, there is a wide spread in the values in the literature, so  $m^*$  becomes in effect a second disposable parameter in addition to the core radius  $r_c$ . It turned out,<sup>2</sup> however, that for lithium and rubidium there is a definite set of values for the two parameters which gives a best fit, and the values of  $m^*$  giving the best agreement were the ones published by Shaw and Smith.<sup>6</sup> The value of  $m^*$  reported for cesium in Table I is obtained by extrapolation.

TABLE I. Values of the Parameters  
Used in the Calculations

	Li	Na	K	Rb	Cs
$a(\text{\AA})$	3.478	4.225	5.225	5.585	6.045
$r_s$	3.236	3.931	4.862	5.197	5.625
$m^*/m$	1.27 <sup>a</sup>	1.0 <sup>b</sup>	0.93 <sup>b</sup>	0.89 <sup>b</sup>	(0.86) <sup>c</sup>
$r_s^*$	4.10	3.931	4.519	4.625	4.84
A	0.999	0.995	1.007	1.008	1.011
B	0.258	0.2625	0.249	0.247	0.242

<sup>a</sup>From Ref. 6.

<sup>b</sup>Values from Ref. 6, as derived from first-order perturbation theory.

<sup>c</sup>Value derived by extrapolation.

### III. NUMERICAL VALUES OF THE INTERIONIC POTENTIAL

The numerical values of the interionic potential (in units of  $10^{-3}$  Ryd), as a function of the interionic  $r$  (in units of the Bohr radius  $a_0$ ), are reported in Tables II-VI. For lithium and rubidium, the tabulation is given for several values of the effective mass  $m^*$ ; for each value of  $m^*$ , we have used the value of the core radius  $r_c$  that gives the best result for the phonon data. The results for cesium are merely for indicative purposes, since only elastic constant data are at present available, and neither  $m^*$  nor  $r_c$  is known with any precision from other data.

Since values for  $r_s$  appropriate to the low-temperature solid have been used, these potentials are only exactly applicable to that case, and slightly different ones should strictly be used for the high-temperature solid and liquid states.

TABLE II. Interionic Potential for Lithium

$r$	$m^*/m = 1.0$ $r_c = 1.320$	$m^*/m = 1.09$ $r_c = 1.356$	$m^*/m = 1.19$ $r_c = 1.386$	$m^*/m = 1.30$ $r_c = 1.415$
3.0	0.125367D 00	0.127673D 00	0.129527D 00	0.131857D 00
3.2	0.976150D-01	0.994373D-01	0.100886D 00	0.102787D 00
3.4	0.751326D-01	0.764866D-01	0.775360D-01	0.790013D-01
3.6	0.570244D-01	0.579482D-01	0.586265D-01	0.596789D-01
3.8	0.425437D-01	0.430888D-01	0.434397D-01	0.441204D-01
4.0	0.310651D-01	0.312885D-01	0.313625D-01	0.317226D-01
4.2	0.220633D-01	0.220233D-01	0.218726D-01	0.219664D-01
4.4	0.150929D-01	0.148462D-01	0.145218D-01	0.144037D-01
4.6	0.977928D-02	0.937791D-02	0.892699D-02	0.864829D-02
4.8	0.580555D-02	0.529660D-02	0.476148D-02	0.436842D-02
5.0	0.290461D-02	0.232902D-02	0.174650D-02	0.127996D-02
5.2	0.853575D-03	0.245944D-03	-0.353294D-03	-0.858772D-03
5.4	-0.534196D-03	-0.114532D-02	-0.173623D-02	-0.225207D-02
5.6	-0.141291D-02	-0.200500D-02	-0.256809D-02	-0.307155D-02
5.8	-0.190874D-02	-0.246465D-02	-0.298557D-02	-0.345949D-02
6.0	-0.212485D-02	-0.263230D-02	-0.310106D-02	-0.353299D-02
6.2	-0.214336D-02	-0.259445D-02	-0.300511D-02	-0.338699D-02
6.4	-0.202939D-02	-0.241982D-02	-0.276973D-02	-0.309717D-02
6.6	-0.183369D-02	-0.216226D-02	-0.245146D-02	-0.272301D-02
6.8	-0.159428D-02	-0.186230D-02	-0.209308D-02	-0.230986D-02
7.0	-0.133960D-02	-0.155025D-02	-0.172648D-02	-0.189142D-02
7.2	-0.108963D-02	-0.124757D-02	-0.137433D-02	-0.149175D-02
7.4	-0.857556D-03	-0.968402D-03	-0.105157D-02	-0.112680D-02
7.6	-0.651758D-03	-0.721692D-03	-0.767495D-03	-0.806321D-03
7.8	-0.476170D-03	-0.511656D-03	-0.526476D-03	-0.534987D-03
8.0	-0.331909D-03	-0.339338D-03	-0.329398D-03	-0.313631D-03
8.2	-0.218035D-03	-0.203558D-03	-0.174718D-03	-0.140399D-03
8.4	-0.131831D-03	-0.101169D-03	-0.588646D-04	-0.113739D-04

TABLE II (Contd.)

$r$	$m^*/m = 1.0$ $r_c = 1.320$	$m^*/m = 1.09$ $r_c = 1.356$	$m^*/m = 1.19$ $r_c = 1.386$	$m^*/m = 1.30$ $r_c = 1.415$
8.6	-0.700200D-04	-0.283114D-04	0.226608D-04	0.785393D-04
8.8	-0.287082D-04	0.195258D-04	0.749962D-04	0.135088D-03
9.0	-0.382384D-05	0.471170D-04	0.103574D-03	0.164323D-03
9.2	0.830139D-05	0.588348D-04	0.113490D-03	0.172067D-03
9.4	0.112931D-04	0.589734D-04	0.109650D-03	0.163832D-03
9.6	0.818777D-05	0.512374D-04	0.963894D-04	0.144577D-03
9.8	0.147738D-05	0.387020D-04	0.773543D-04	0.118545D-03
10.0	-0.665466D-05	0.240759D-04	0.557074D-04	0.893470D-04
10.2	-0.147633D-04	0.926979D-05	0.338127D-04	0.598202D-04
10.4	-0.217293D-04	-0.423824D-05	0.134748D-04	0.321162D-04
10.6	-0.268134D-04	-0.154054D-04	-0.400711D-05	0.779248D-05
10.8	-0.297921D-04	-0.237893D-04	-0.179654D-04	-0.122310D-04
11.0	-0.305185D-04	-0.291081D-04	-0.280204D-04	-0.274694D-04
11.2	-0.291852D-04	-0.314624D-04	-0.341908D-04	-0.378518D-04
11.4	-0.261508D-04	-0.311969D-04	-0.367981D-04	-0.436572D-04
11.6	-0.217287D-04	-0.286521D-04	-0.362381D-04	-0.453409D-04
11.8	-0.164512D-04	-0.244185D-04	-0.331408D-04	-0.435636D-04
12.0	-0.107371D-04	-0.190201D-04	-0.281372D-04	-0.390598D-04
12.2	-0.496861D-05	-0.129483D-04	-0.218373D-04	-0.325684D-04
12.4	0.413199D-06	-0.677137D-05	-0.149120D-04	-0.248580D-04
12.6	0.519119D-05	-0.843635D-06	-0.786612D-05	-0.165958D-04
12.8	0.912222D-05	0.447156D-05	-0.117583D-05	-0.838109D-05
13.0	0.120462D-04	0.888907D-05	0.476055D-05	-0.728267D-06
13.2	0.139757D-04	0.123148D-04	0.972532D-05	0.600184D-05
13.4	0.148583D-04	0.146110D-04	0.135096D-04	0.115229D-04
13.6	0.147974D-04	0.158022D-04	0.160522D-04	0.156768D-04
13.8	0.139342D-04	0.159813D-04	0.173862D-04	0.184204D-04
14.0	0.123631D-04	0.152087D-04	0.175487D-04	0.197638D-04
14.2	0.103166D-04	0.136974D-04	0.167131D-04	0.198275D-04
14.4	0.794452D-05	0.116034D-04	0.150410D-04	0.187707D-04
14.6	0.540526D-05	0.909625D-05	0.127125D-04	0.167833D-04
14.8	0.291053D-05	0.641441D-05	0.997389D-05	0.141087D-04
15.0	0.545892D-06	0.368200D-05	0.699497D-05	0.109654D-04
15.2	-0.154586D-05	0.107814D-05	0.398134D-05	0.758492D-05
15.4	-0.326781D-05	-0.125259D-05	0.111694D-05	0.418850D-05
15.6	-0.460908D-05	-0.325542D-05	-0.149010D-05	0.946452D-06
15.8	-0.549483D-05	-0.481576D-05	-0.369825D-05	-0.197232D-05
16.0	-0.595508D-05	-0.592115D-05	-0.544682D-05	-0.445260D-05
16.2	-0.602427D-05	-0.657636D-05	-0.670568D-05	-0.641995D-05
16.4	-0.570979D-05	-0.676207D-05	-0.743633D-05	-0.781486D-05
16.6	-0.511719D-05	-0.656277D-05	-0.768779D-05	-0.864015D-05
16.8	-0.428933D-05	-0.601352D-05	-0.748850D-05	-0.891202D-05
17.0	-0.329523D-05	-0.517659D-05	-0.689193D-05	-0.867172D-05

TABLE II (Contd.)

	$m^*/m = 1.0$ $r_c = 1.320$	$m^*/m = 1.09$ $r_c = 1.356$	$m^*/m = 1.19$ $r_c = 1.386$	$m^*/m = 1.30$ $r_c = 1.415$
17.2	-0.224267D-05	-0.416315D-05	-0.599893D-05	-0.800023D-05
17.4	-0.116066D-05	-0.301290D-05	-0.486504D-05	-0.696854D-05
17.6	-0.138208D-06	-0.182556D-05	-0.359094D-05	-0.567410D-05
17.8	0.768928D-06	-0.676979D-06	-0.226678D-05	-0.421749D-05
18.0	0.154885D-05	0.401533D-06	-0.948068D-06	-0.268159D-05
18.2	0.213550D-05	0.132418D-05	0.271092D-06	-0.116578D-05
18.4	0.253885D-05	0.207701D-05	0.134878D-05	0.257275D-06
18.6	0.275683D-05	0.264005D-05	0.224630D-05	0.152612D-05
18.8	0.277230D-05	0.297746D-05	0.291543D-05	0.258041D-05
19.0	0.263771D-05	0.312513D-05	0.336572D-05	0.339639D-05
19.2	0.235397D-05	0.307440D-05	0.358213D-05	0.394999D-05
19.4	0.195259D-05	0.284648D-05	0.357371D-05	0.423519D-05
19.6	0.148939D-05	0.249342D-05	0.337966D-05	0.427136D-05
19.8	0.967192D-06	0.201839D-05	0.300809D-05	0.407095D-05
20.0	0.443047D-06	0.147910D-05	0.250903D-05	0.367162D-05
20.2	-0.545990D-07	0.911619D-06	0.192281D-05	0.311451D-05
20.4	-0.518420D-06	0.330855D-06	0.127448D-05	0.243554D-05
20.6	-0.897849D-06	-0.203456D-06	0.623443D-06	0.168976D-05
20.8	-0.120009D-05	-0.685459D-06	-0.814584D-08	0.916773D-06
21.0	-0.141238D-05	-0.109235D-05	-0.588772D-06	0.157839D-06
21.2	-0.151496D-05	-0.139220D-05	-0.107944D-05	-0.542294D-06
21.4	-0.153732D-05	-0.160295D-05	-0.147981D-05	-0.116064D-05
21.6	-0.146541D-05	-0.170262D-05	-0.176413D-05	-0.166708D-05
21.8	-0.131562D-05	-0.169816D-05	-0.192821D-05	-0.204425D-05

TABLE III. Interionic Potential for Sodium

	$m^*/m = 1.0$ $r_c = 1.694$	$m^*/m = 1.0$ $r_c = 1.694$	$m^*/m = 1.0$ $r_c = 1.694$
3.0	0.197407D 00	5.2	0.151283D-01
3.2	0.164152D 00	5.4	0.105371D-01
3.4	0.135798D 00	5.6	0.688875D-02
3.6	0.111627D 00	5.8	0.403545D-02
3.8	0.910763D-01	6.0	0.184745D-02
4.0	0.736638D-01	6.2	0.211625D-03
4.2	0.589736D-01	6.4	-0.970350D-03
4.4	0.466437D-01	6.6	-0.178838D-02
4.6	0.363571D-01	6.8	-0.230216D-02
4.8	0.278344D-01	7.0	-0.258788D-02
5.0	0.208303D-01	7.2	-0.269425D-02

TABLE III (Contd.)

$r$	$m^*/m = 1.0$ $r_c = 1.694$	$r$	$m^*/m = 1.0$ $r_c = 1.694$	$r$	$m^*/m = 1.0$ $r_c = 1.694$
9.6	-0.336937D-03	13.8	-0.334601D-04	18.0	0.888042D-05
9.8	-0.212183D-03	14.0	-0.338483D-04	18.2	0.676745D-05
10.0	-0.111673D-03	14.2	-0.325283D-04	18.4	0.460162D-05
10.2	-0.334600D-04	14.4	-0.298276D-04	18.6	0.247995D-05
10.4	0.246896D-04	14.6	-0.260389D-04	18.8	0.462115D-06
10.6	0.652547D-04	14.8	-0.214779D-04	19.0	-0.138445D-05
10.8	0.908773D-04	15.0	-0.164748D-04	19.2	-0.299400D-05
11.0	0.104101D-03	15.2	-0.112919D-04	19.4	-0.434155D-05
11.2	0.107350D-03	15.4	-0.616537D-05	19.6	-0.540655D-05
11.4	0.102962D-03	15.6	-0.133188D-05	19.8	-0.616199D-05
11.6	0.930159D-04	15.8	0.304405D-05	20.0	-0.661595D-05
11.8	0.793077D-04	16.0	0.685077D-05	20.2	-0.678917D-05
12.0	0.634519D-04	16.2	0.997746D-05	20.4	-0.668839D-05
12.2	0.467888D-04	16.4	0.123695D-04	20.6	-0.634351D-05
12.4	0.303469D-04	16.6	0.140322D-04	20.8	-0.580154D-05
12.6	0.149705D-04	16.8	0.149674D-04	21.0	-0.509063D-05
12.8	0.129352D-05	17.0	0.152059D-04	21.2	-0.424759D-05
13.0	-0.103132D-04	17.2	0.148321D-04	21.4	-0.332750D-05
13.2	-0.196216D-04	17.4	0.139218D-04	21.6	-0.236577D-05
13.4	-0.265207D-04	17.6	0.125511D-04	21.8	-0.139261D-05
13.6	-0.310804D-04	17.8	0.108356D-04		

TABLE IV. Interionic Potential for Potassium

$r$	$m^*/m = 0.93$ $r_c = 2.226$	$r$	$m^*/m = 0.93$ $r_c = 2.226$	$r$	$m^*/m = 0.93$ $r_c = 2.226$
3.0	0.278457D 00	5.8	0.308242D-01	8.6	-0.2225948D-02
3.2	0.242640D 00	6.0	0.249795D-01	8.8	-0.243939D-02
3.4	0.211534D 00	6.2	0.199512D-01	9.0	-0.251721D-02
3.6	0.184327D 00	6.4	0.156515D-01	9.2	-0.251322D-02
3.8	0.160390D 00	6.6	0.119999D-01	9.4	-0.244516D-02
4.0	0.139232D 00	6.8	0.892274D-02	9.6	-0.232831D-02
4.2	0.120473D 00	7.0	0.635243D-02	9.8	-0.217577D-02
4.4	0.103818D 00	7.2	0.422753D-02	10.0	-0.199870D-02
4.6	0.890413D-01	7.4	0.249219D-02	10.2	-0.180649D-02
4.8	0.759603D-01	7.6	0.109570D-02	10.4	-0.160693D-02
5.0	0.644149D-01	7.8	-0.790817D-05	10.6	-0.140636D-02
5.2	0.542582D-01	8.0	-0.860027D-03	10.8	-0.120989D-02
5.4	0.453549D-01	8.2	-0.149776D-02	11.0	-0.102152D-02
5.6	0.375812D-01	8.4	-0.195436D-02	11.2	-0.844283D-03

TABLE IV (Contd.)

$r$	$m^*/m = 0.93$ $r_c = 2.226$	$r$	$m^*/m = 0.93$ $r_c = 2.226$	$r$	$m^*/m = 0.93$ $r_c = 2.226$
11.4	-0.680339D-03	15.0	0.103600D-03	18.6	-0.327174D-04
11.6	-0.531143D-03	15.2	0.862432D-04	18.8	-0.285396D-04
11.8	-0.397551D-03	15.4	0.687257D-04	19.0	-0.239767D-04
12.0	-0.279897D-03	15.6	0.515845D-04	19.2	-0.191911D-04
12.2	-0.178071D-03	15.8	0.352536D-04	19.4	-0.143277D-04
12.4	-0.916262D-04	16.0	0.200809D-04	19.6	-0.951917D-05
12.6	-0.198590D-04	16.2	0.633847D-05	19.8	-0.488726D-05
12.8	0.381480D-04	16.4	-0.578087D-05	20.0	-0.535314D-06
13.0	0.834779D-04	16.6	-0.161618D-04	20.2	0.345536D-05
13.2	0.117310D-03	16.8	-0.247489D-04	20.4	0.701895D-05
13.4	0.140872D-03	17.0	-0.315342D-04	20.6	0.101021D-04
13.6	0.155416D-03	17.2	-0.365592D-04	20.8	0.126698D-04
13.8	0.162202D-03	17.4	-0.399111D-04	21.0	0.147069D-04
14.0	0.162450D-03	17.6	-0.417074D-04	21.2	0.162107D-04
14.2	0.157316D-03	17.8	-0.420839D-04	21.4	0.171877D-04
14.4	0.147802D-03	18.0	-0.411969D-04	21.6	0.176576D-04
14.6	0.135198D-03	18.2	-0.392211D-04	21.8	0.176542D-04
14.8	0.120161D-03	18.4	-0.363362D-04		

TABLE V. Interionic Potential for Rubidium

$r$	$m^*/m = 1.0$ $r_c = 2.47$	$r$	$m^*/m = 0.89$ $r_c = 2.45$	$r$	$m^*/m = 0.82$ $r_c = 2.43$
3.0	0.301918D 00		0.303186D 00		0.303692D 00
3.2	0.265921D 00		0.266876D 00		0.267185D 00
3.4	0.234608D 00		0.235295D 00		0.235436D 00
3.6	0.207151D 00		0.207616D 00		0.207619D 00
3.8	0.182902D 00		0.183192D 00		0.183088D 00
4.0	0.161355D 00		0.161515D 00		0.161333D 00
4.2	0.142110D 00		0.142183D 00		0.141953D 00
4.4	0.124849D 00		0.124877D 00		0.124625D 00
4.6	0.109323D 00		0.109343D 00		0.109096D 00
4.8	0.953421D-01		0.953858D-01		0.951663D-01
5.0	0.827582D-01		0.828524D-01		0.826796D-01
5.2	0.714569D-01		0.716200D-01		0.715073D-01
5.4	0.613395D-01		0.615815D-01		0.615366D-01
5.6	0.523141D-01		0.526377D-01		0.526629D-01
5.8	0.442923D-01		0.446949D-01		0.447889D-01
6.0	0.371899D-01		0.376654D-01		0.378245D-01
6.2	0.309282D-01		0.314684D-01		0.316870D-01

TABLE V (Contd.)

$r$	$m^*/m = 1.0$ $r_c = 2.47$	$m^*/m = 0.89$ $r_c = 2.45$	$m^*/m = 0.82$ $r_c = 2.43$
6.4	0.254336D-01	0.260285D-01	0.262998D-01
6.6	0.206365D-01	0.212751D-01	0.215915D-01
6.8	0.164713D-01	0.171425D-01	0.174960D-01
7.0	0.128766D-01	0.135696D-01	0.139525D-01
7.2	0.979586D-02	0.105001D-01	0.109047D-01
7.4	0.717594D-02	0.788173D-02	0.830068D-02
7.6	0.496747D-02	0.566586D-02	0.609236D-02
7.8	0.312471D-02	0.380783D-02	0.423571D-02
8.0	0.160566D-02	0.226666D-02	0.269036D-02
8.2	0.371743D-03	0.100474D-02	0.141936D-02
8.4	-0.612604D-03	-0.124499D-04	0.388854D-03
8.6	-0.137996D-02	-0.816461D-03	-0.432011D-03
8.8	-0.195986D-02	-0.143586D-02	-0.107114D-02
9.0	-0.237899D-02	-0.189648D-02	-0.155380D-02
9.2	-0.266152D-02	-0.222173D-02	-0.190283D-02
9.4	-0.282932D-02	-0.243270D-02	-0.213876D-02
9.6	-0.290190D-02	-0.254823D-02	-0.227993D-02
9.8	-0.289651D-02	-0.258502D-02	-0.234265D-02
10.0	-0.282846D-02	-0.255793D-02	-0.234138D-02
10.2	-0.271130D-02	-0.248008D-02	-0.228892D-02
10.4	-0.255690D-02	-0.236298D-02	-0.219646D-02
10.6	-0.237546D-02	-0.221656D-02	-0.207370D-02
10.8	-0.217570D-02	-0.204938D-02	-0.192903D-02
11.0	-0.196515D-02	-0.186883D-02	-0.176966D-02
11.2	-0.175015D-02	-0.168114D-02	-0.160171D-02
11.4	-0.153594D-02	-0.149150D-02	-0.143026D-02
11.6	-0.132671D-02	-0.130414D-02	-0.125951D-02
11.8	-0.112585D-02	-0.112250D-02	-0.109288D-02
12.0	-0.936070D-03	-0.949328D-03	-0.933118D-03
12.2	-0.759328D-03	-0.786696D-03	-0.782291D-03
12.4	-0.596959D-03	-0.636070D-03	-0.641923D-03
12.6	-0.449803D-03	-0.498442D-03	-0.513072D-03
12.8	-0.318323D-03	-0.374423D-03	-0.396409D-03
13.0	-0.202610D-03	-0.264251D-03	-0.292243D-03
13.2	-0.102386D-03	-0.167825D-03	-0.200565D-03
13.4	-0.171103D-04	-0.847928D-04	-0.121128D-03
13.6	0.539060D-04	-0.146346D-04	-0.535079D-04
13.8	0.111489D-03	0.433194D-04	0.287656D-05
14.0	0.156628D-03	0.898929D-04	0.487465D-04
14.2	0.190423D-03	0.126011D-03	0.849178D-04
14.4	0.213986D-03	0.152633D-03	0.112247D-03

TABLE V (Contd.)

$r$	$m^*/m = 1.0$ $r_c = 2.47$	$m^*/m = 0.89$ $r_c = 2.45$	$m^*/m = 0.82$ $r_c = 2.43$
14.6	0.228418D-03	0.170725D-03	0.131618D-03
14.8	0.234846D-03	0.181287D-03	0.143939D-03
15.0	0.234415D-03	0.185330D-03	0.150127D-03
15.2	0.228218D-03	0.183825D-03	0.151068D-03
15.4	0.217256D-03	0.177679D-03	0.147597D-03
15.6	0.202477D-03	0.167757D-03	0.140515D-03
15.8	0.184801D-03	0.154892D-03	0.130587D-03
16.0	0.165072D-03	0.139849D-03	0.118512D-03
16.2	0.144020D-03	0.123303D-03	0.104918D-03
16.4	0.122285D-03	0.105851D-03	0.903645D-04
16.6	0.100458D-03	0.880459D-04	0.753602D-04
16.8	0.790693D-04	0.703719D-04	0.603525D-04
17.0	0.585371D-04	0.532269D-04	0.457111D-04
17.2	0.391870D-04	0.369286D-04	0.317381D-04
17.4	0.212950D-04	0.217463D-04	0.186876D-04
17.6	0.509515D-05	0.790353D-05	0.676508D-05
17.8	-0.925698D-05	-0.444482D-05	-0.388418D-05
18.0	-0.216892D-04	-0.152119D-04	-0.131716D-04
18.2	-0.321705D-04	-0.243498D-04	-0.210455D-04
18.4	-0.406873D-04	-0.318344D-04	-0.274822D-04
18.6	-0.472690D-04	-0.376822D-04	-0.324957D-04
18.8	-0.520062D-04	-0.419586D-04	-0.361392D-04
19.0	-0.550202D-04	-0.447557D-04	-0.384888D-04
19.2	-0.564300D-04	-0.461702D-04	-0.396303D-04
19.4	-0.563642D-04	-0.463124D-04	-0.396643D-04
19.6	-0.549878D-04	-0.453205D-04	-0.387124D-04
19.8	-0.524866D-04	-0.433481D-04	-0.369073D-04
20.0	-0.490316D-04	-0.405406D-04	-0.343775D-04
20.2	-0.447789D-04	-0.370355D-04	-0.312482D-04
20.4	-0.398972D-04	-0.329796D-04	-0.276503D-04
20.6	-0.345684D-04	-0.285267D-04	-0.237173D-04
20.8	-0.289558D-04	-0.238164D-04	-0.195709D-04
21.0	-0.231928D-04	-0.189673D-04	-0.153182D-04
21.2	-0.174071D-04	-0.140932D-04	-0.110611D-04
21.4	-0.117342D-04	-0.930967D-05	-0.689914D-05
21.6	-0.629354D-05	-0.471789D-05	-0.291837D-05
21.8	-0.117023D-05	-0.393654D-06	0.814099D-06

TABLE VI. Interionic Potential for Cesium

$r$	$m^*/m = 1.0$ $r_c = 2.70$	$m^*/m = 0.85$ $r_c = 2.65$	$m^*/m = 0.78$ $r_c = 2.60$
3.0	0.324383D 00	0.324647D 00	0.323030D 00
3.2	0.287979D 00	0.287778D 00	0.285943D 00
3.4	0.256300D 00	0.255685D 00	0.253659D 00
3.6	0.228509D 00	0.227535D 00	0.225349D 00
3.8	0.203949D 00	0.202673D 00	0.200358D 00
4.0	0.182099D 00	0.180580D 00	0.178169D 00
4.2	0.162542D 00	0.160840D 00	0.158368D 00
4.4	0.144948D 00	0.143121D 00	0.140622D 00
4.6	0.129048D 00	0.127154D 00	0.124663D 00
4.8	0.114630D 00	0.112723D 00	0.110272D 00
5.0	0.101523D 00	0.0996551D-01	0.972768D-01
5.2	0.895952D-01	0.878124D-01	0.855387D-01
5.4	0.787432D-01	0.770878D-01	0.749462D-01
5.6	0.688883D-01	0.673927D-01	0.654049D-01
5.8	0.599641D-01	0.586498D-01	0.568296D-01
6.0	0.519090D-01	0.507867D-01	0.491411D-01
6.2	0.446627D-01	0.437347D-01	0.422651D-01
6.4	0.381661D-01	0.374286D-01	0.361330D-01
6.6	0.323628D-01	0.318078D-01	0.306812D-01
6.8	0.271995D-01	0.268157D-01	0.258506D-01
7.0	0.226254D-01	0.223990D-01	0.215861D-01
7.2	0.185918D-01	0.185075D-01	0.178362D-01
7.4	0.150523D-01	0.150941D-01	0.145535D-01
7.6	0.119632D-01	0.121151D-01	0.116936D-01
7.8	0.928384D-02	0.952965D-02	0.921561D-02
8.0	0.697559D-02	0.729962D-02	0.708141D-02
8.2	0.500210D-02	0.538944D-02	0.525575D-02
8.4	0.332935D-02	0.376610D-02	0.370611D-02
8.6	0.192588D-02	0.239917D-02	0.240257D-02
8.8	0.762548D-03	0.126054D-02	0.131754D-02
9.0	-0.187814D-03	0.324184D-03	0.425650D-03
9.2	-0.950441D-03	-0.433892D-03	-0.296356D-03
9.4	-0.154848D-02	-0.103561D-02	-0.869658D-03
9.6	-0.200301D-02	-0.150094D-02	-0.131354D-02
9.8	-0.233327D-02	-0.184809D-02	-0.164556D-02
10.0	-0.255694D-02	-0.209371D-02	-0.188164D-02
10.2	-0.269011D-02	-0.225284D-02	-0.203613D-02
10.4	-0.274721D-02	-0.233899D-02	-0.212188D-02
10.6	-0.274109D-02	-0.236424D-02	-0.215040D-02
10.8	-0.268833D-02	-0.233943D-02	-0.213198D-02
11.0	-0.258427D-02	-0.227424D-02	-0.207575D-02
11.2	-0.245315D-02	-0.217724D-02	-0.198973D-02
11.4	-0.229791D-02	-0.205587D-02	-0.188094D-02
11.6	-0.212547D-02	-0.191663D-02	-0.175551D-02
11.8	-0.194187D-02	-0.176519D-02	-0.161872D-02
12.0	-0.175237D-02	-0.160645D-02	-0.147511D-02
12.2	-0.156138D-02	-0.144455D-02	-0.132852D-02
12.4	-0.137250D-02	-0.128290D-02	-0.118213D-02

TABLE VI (Contd.)

$r$	$m^*/m = 1.0$ $r_c = 2.70$	$m^*/m = 0.85$ $r_c = 2.65$	$m^*/m = 0.78$ $r_c = 2.60$
12.6	-0.118870D-02	-0.112436D-02	-0.103859D-02
12.8	-0.101245D-02	-0.971276D-03	-0.900036D-03
13.0	-0.845726D-03	-0.825516D-03	-0.768163D-03
13.2	-0.689945D-03	-0.688482D-03	-0.644245D-03
13.4	-0.546079D-03	-0.561177D-03	-0.529205D-03
13.6	-0.414787D-03	-0.444307D-03	-0.423676D-03
13.8	-0.296479D-03	-0.338318D-03	-0.328030D-03
14.0	-0.191278D-03	-0.248389D-03	-0.242398D-03
14.2	-0.990087D-04	-0.159454D-03	-0.166712D-03
14.4	-0.192941D-04	-0.862739D-04	-0.100746D-03
14.6	0.483352D-04	-0.234946D-04	-0.441586D-04
14.8	0.104442D-03	0.293415D-04	0.350191D-05
15.0	0.149734D-03	0.728134D-04	0.427786D-04
15.2	0.185036D-03	0.107591D-03	0.742798D-04
15.4	0.211207D-03	0.134378D-03	0.986461D-04
15.6	0.229077D-03	0.153881D-03	0.116536D-03
15.8	0.239490D-03	0.166825D-03	0.128625D-03
16.0	0.243338D-03	0.173970D-03	0.135597D-03
16.2	0.241524D-03	0.176068D-03	0.138123D-03
16.4	0.234883D-03	0.173831D-03	0.136844D-03
16.6	0.224179D-03	0.167926D-03	0.132369D-03
16.8	0.210158D-03	0.159000D-03	0.125282D-03
17.0	0.193560D-03	0.147684D-03	0.116135D-03
17.2	0.175073D-03	0.134557D-03	0.105434D-03
17.4	0.155284D-03	0.120130D-03	0.936311D-04
17.6	0.134707D-03	0.104859D-03	0.811364D-04
17.8	0.113837D-03	0.891745D-04	0.683219D-04
18.0	0.931382D-04	0.734650D-04	0.555155D-04
18.2	0.729927D-04	0.580584D-04	0.429941D-04
18.4	0.536926D-04	0.432160D-04	0.309862D-04
18.6	0.354827D-04	0.291601D-04	0.196837D-04
18.8	0.185939D-04	0.160885D-04	0.924567D-05
19.0	0.321731D-05	0.415916D-05	-0.207675D-06
19.2	-0.105339D-04	-0.652688D-05	-0.859640D-05
19.4	-0.226093D-04	-0.159128D-04	-0.158728D-04
19.6	-0.329739D-04	-0.239606D-04	-0.220113D-04
19.8	-0.415975D-04	-0.306473D-04	-0.270079D-04
20.0	-0.484903D-04	-0.359831D-04	-0.308842D-04
20.2	-0.537212D-04	-0.400176D-04	-0.336862D-04
20.4	-0.573857D-04	-0.428190D-04	-0.354738D-04
20.6	-0.595692D-04	-0.444558D-04	-0.363140D-04
20.8	-0.603577D-04	-0.450037D-04	-0.362838D-04
21.0	-0.598713D-04	-0.445613D-04	-0.354731D-04
21.2	-0.582630D-04	-0.432458D-04	-0.339798D-04
21.4	-0.556806D-04	-0.411719D-04	-0.319009D-04
21.6	-0.522477D-04	-0.384428D-04	-0.293305D-04
21.8	-0.480891D-04	-0.351641D-04	-0.263640D-04

## REFERENCES

1. K. Singwi, A. Sjölander, M. P. Tosi, and R. H. Land, *Electron Correlations at Metallic Densities, IV*, Phys. Rev. B1, 1044 (1970).
2. D. L. Price, K. S. Singwi, and M. P. Tosi, *Lattice Dynamics of Alkali Metals in the Self-Consistent Screening Theory*, Phys. Rev. B2, 2983 (1970).
3. N. W. Ashcroft, *Electron-Ion Pseudopotentials in Metals*, Phys. Lett. 23, 48 (1966).
4. Wei-Mei Shyu, K. S. Singwi, and M. P. Tosi, *Many-Electron Correlation Effects on the Metallic Interionic Potential*, Phys. Rev. (in press).
5. W. Cochran, *Lattice Dynamics of Sodium*, Proc. Roy. Soc. A276, 308 (1963).
6. R. W. Shaw and N. V. Smith, *Model-Potential Calculation of the Density of States in Liquid and Solid Lithium, Cadmium, and Indium*, Phys. Rev. 178, 985 (1969).



X  
ARGONNE NATIONAL LAB WEST



3 4444 00010989 2

